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Optimal guidance law in quantum mechanics



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HIGHLIGHTS

- Treating quantum mechanics as a pursuit-evasion game.
- Reveal an interesting analogy between guided flight motion and guided quantum motion.
- Solve optimal quantum guidance problem by dynamic programming.
- Gives a formal proof of de Broglie–Bohm's idea of a pilot wave.
- The optimal pilot wave is shown to be a wavefunction solved from Schrödinger equation.

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ABSTRACT

Following de Broglie's idea of a pilot wave, this paper treats quantum mechanics as a problem of stochastic optimal guidance law design. The guidance scenario considered in the quantum world is that an electron is the flight vehicle to be guided and its accompanying pilot wave is the guidance law to be designed so as to guide the electron to a random target driven by the Wiener process, while minimizing a cost-to-go function. After solving the stochastic optimal guidance problem by differential dynamic programming, we point out that the optimal pilot wave guiding the particle's motion is just the wavefunction $\Psi(t, \mathbf{x})$, a solution to the Schrödinger equation; meanwhile, the closed-loop guidance system forms a complex state-space dynamics for $\Psi(t, \mathbf{x})$, from which quantum operators emerge naturally. Quantum trajectories under the action of the optimal guidance law are solved and their statistical distribution is shown to coincide with the prediction of the probability density function $\Psi^*\Psi$.

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1. Introduction

The subject of stochastic optimal guidance in aerospace is concerned with determining control policies which optimize some probabilistic measure of performance for flight vehicles [1,2]. From the viewpoint of optimal guidance law design, this paper aims to reveal an interesting analogy between guided flight motion and guided quantum motion by showing that both can be described by the same pursuit–evasion game. The idea of a “pilot wave” that guides the movement of an electron was first suggested by de Broglie at the 1927 Solvay Congress. According to de Broglie’s idea, electrons have a dual particle–wave nature. Accompanying every electron is a wave, which guides, or “pilots”, the electron through space. After de Broglie’s initiation, a substantial development of the pilot wave began with Bohm, who pointed out that the action of a pilot wave is like that of radio wave guiding a ship. With the observation that the ship is moving with its own energy, and that the form of the radio waves is taken up to direct the much greater energy of the ship, Bohm proposed that an electron moves under its own energy, and that the pilot wave guides the energy of the electron. There are three main postulates in Bohm’s proposal [3]:

- (1) An individual physical system comprises a wave propagating in space and time together with a point particle which moves continuously under the guidance of the wave.
- (2) The wave is mathematically described by $\Psi(t, \mathbf{x})$, a solution to the Schrödinger equation.
- (3) The particle motion is obtained as the solution $\mathbf{x}(t)$ to the equation

$$\dot{\mathbf{x}} = (1/m)\nabla S_B(\mathbf{x}, t), \quad (1.1)$$

where S_B is the phase of $\Psi = R_B(t, \mathbf{x})e^{iS_B(t,\mathbf{x})/\hbar}$, $R_B, S_B \in \mathbf{R}$.

Eq. (1.1) was known as the guidance condition of quantum motion. It was recognized [4] later that Eq. (1.1) only represents some regular velocity $\bar{\mathbf{v}} = \nabla S_B/m$, while the actual velocity $\mathbf{v} = \bar{\mathbf{v}} + \xi(t)$ has an additional random component $\xi(t)$. An explicit characterization of the random velocity $\xi(t)$ was derived by Bohm and Hiley [5]:

$$\mathbf{v} = \bar{\mathbf{v}} + \xi(t) = \frac{\nabla S_B}{m} + v \frac{\nabla R_B}{R_B}, \quad (1.2)$$

where v is a diffusion coefficient. This random velocity $\xi(t)$ is actually the osmotic velocity originating from the Brownian motion. The similarities between quantum mechanics and Brownian motion were first noted by Fürth [6] and developed by Kershaw [7], Nelson [8], Comisar [9] and Rosenstein [10]. Nelson [8] proposed a Brownian model for quantum motion:

$$d\mathbf{x} = \mathbf{b}(t, \mathbf{x})dt + d\mathbf{w}, \quad (1.3)$$

which comprises a drift component $\mathbf{b}(t, \mathbf{x})dt$ and a diffusion component described by the Wiener process $d\mathbf{w}$ with variance $E(dw_i dw_j) = 2v\delta_{ij}dt$. It can be shown that Nelson’s drift velocity $\mathbf{b}(t, \mathbf{x})$ is identical to the velocity \mathbf{v} given by Eq. (1.2). Nelson gave a stochastic interpretation of the Schrödinger equation by showing that the classical equations of motion for a particle undergoing a Brownian motion with drift velocity $\mathbf{b}(t, \mathbf{x})$ given by Eq. (1.2) lead naturally to the Schrödinger equation, if the diffusion coefficient v is chosen as $v = \hbar/2m$.

On the other hand, Comisar [9] connected Brownian motion to the path integral and represented the wavefunction as a sum of path integrals over Brownian-motion trajectories. By the analogy between the free-particle propagator and the Brownian-motion Green function, Fürth [6] and Comisar [9] pointed out that the path-integral approach and the Brownian-motion approach to quantum mechanics are equivalent, if the diffusion coefficient v is chosen as $v = i\hbar/2m$, which has an additional imaginary factor $i = \sqrt{-1}$, as compared to $v = \hbar/2m$ suggested by Bohm and Nelson. Based on this imaginary diffusion coefficient, Comisar [9] proposed a complex Langevin equation to describe quantum velocity

$$d\mathbf{v} = -\beta\mathbf{v}dt + i^{1/2}d\mathbf{w}. \quad (1.4)$$

Due to the presence of the complex coefficient $i^{1/2} = (-1 + i)/\sqrt{2}$, which also appears in our later derivation, Comisar concluded that the randomizing process in quantum mechanics involves fictitious

collisions described by trajectories in a phase space with complex velocity \mathbf{v} . It can be said that the optimal quantum guidance law addressed in this paper inherits the idea of guiding wave from Bohm [3], and adopts the randomizing process proposed by Nelson [8], while confirming the complexifying process proposed by Comisar [9].

Inspired by the fact that classical mechanics can be derived by the principle of least action [11] and hence by the optimal control theory [2], we aim to show that the de Broglie–Bohm guided-wave approach to quantum mechanics can be recast into an optimal guidance law design problem. The equivalent guidance scenario taking place in the quantum world is that an electron is the flight vehicle to be guided and its accompanying pilot wave is the optimal guidance law to be designed so as to guide the electron to a random target driven by a Wiener process, while minimizing a prescribed cost function.

An optimal guidance problem can be solved either by the variational approach or by the dynamic programming approach, but only the latter is applicable to both deterministic and stochastic systems. Although the variational approach had been employed to derive the deterministic wave equation by Schrödinger himself [12], it is unable to provide us with the stochastic differential equations describing the particle's quantum motion accompanying the wave. For the latter purpose, the dynamic programming approach to optimal control becomes the only workable method. Here we will show that the stochastic Hamilton–Jacobi–Bellman (HJB) equation arising from the dynamic programming approach [13] to optimal stochastic control is just the Schrödinger equation, whose solution $\Psi(t, x)$ determines the optimal pilot wave guiding a particle's quantum motion. Our result gives a formal proof of the role of a wavefunction $\Psi(t, x)$ as a guiding wave and provides necessary corrections to the Bohm's postulates listed above. On the other hand, the obtained closed-loop dynamics under the action of the optimal guidance laws is shown to yield a complex dynamical representation of the wavefunction $\Psi(t, x)$, which reveals the internal mechanism underlying the externally observed probability density function $\Psi^*\Psi$.

The remaining sections are organized as follows. Section 2 introduces a unified optimal control formulation of classical and quantum mechanics by the dynamic programming approach. In Section 3, we demonstrate that the quantum motion of a particle is guided by its accompanying pilot wave in an optimal manner that minimizes the Lagrangian cost function in the presence of a stochastic Wiener process. The optimal pilot wave is found to be a wavefunction $\Psi(t, \mathbf{x})$ solved from the Schrödinger equation. In Section 4, we show that quantum Hamilton mechanics [14] proposed in the literature can be derived from the stochastic optimal control approach, just as classical Hamilton mechanics can be derived from the deterministic optimal control approach. The optimal quantum trajectories in the presence of Gaussian white noise are computed in Section 5, where we show that the deviation of the quantum trajectories from their mean trajectory satisfies the uncertainty principle. The consistency of the optimal quantum guidance formulation with orthodox quantum mechanics is demonstrated in Section 6, where the statistical distribution of an ensemble of random trajectories computed from Section 5 is shown to reproduce the probability density functions $\Psi^*(t, x)\Psi(t, x)$ exactly.

2. Optimal control approach to classical and quantum mechanics

In this section we will survey the optimal control approach to classical mechanics and examine its applicability to quantum mechanics. It is well known that classical mechanics can be formulated as an optimal control problem, which has been solved in two different ways: the variational approach and the dynamic programming approach. We first give a brief review of the two approaches and then consider their validity in quantum mechanics. Parallel to the situation that the variational approach was employed to give an optimal control formulation of classical mechanics, we find that the dynamic programming approach can be employed to give an optimal control formulation of quantum mechanics.

Consider a dynamical system described by the set of differential equations,

$$\dot{\mathbf{x}} = f(t, \mathbf{x}, \mathbf{u}), \quad \mathbf{x}(t_0) = \mathbf{x}_0 \quad (2.1)$$

where \mathbf{x} is the state vector and \mathbf{u} is the control vector, which is to be determined to minimize the following cost function,

$$J(t_0, \mathbf{x}_0, \mathbf{u}) = \int_{t_0}^{t_f} L(\tau, \mathbf{x}(\tau), \mathbf{u}(\tau)) d\tau, \quad (2.2)$$

where $L(\tau, \mathbf{x}(\tau), \mathbf{u}(\tau))$ is the instantaneous cost rate. Classical mechanics can be converted into the above optimal control problem by choosing $L(\tau, \mathbf{x}(\tau), \mathbf{u}(\tau))$ as the Lagrangian of the system and choosing $f(t, \mathbf{x}, \mathbf{u}) = \mathbf{u}$. In other words, classical mechanics is itself an optimal control design wherein an optimal velocity $\mathbf{u} = \dot{\mathbf{x}}$ is determined automatically so as to minimize the cost function $J(t_0, \mathbf{x}_0, \mathbf{u})$. The accompanying Hamiltonian is defined as

$$H(t, \mathbf{x}, \mathbf{u}, \mathbf{p}) = \mathbf{p}^T \dot{\mathbf{x}} - L(t, \mathbf{x}, \mathbf{u}) = \mathbf{p}^T \mathbf{u} - L(t, \mathbf{x}, \mathbf{u}), \quad (2.3)$$

where \mathbf{p} is a Lagrange multiplier to be determined. The variational approach gives the optimal control law as

$$\frac{\partial H}{\partial \mathbf{u}} = 0 \Rightarrow \mathbf{p} = \frac{\partial L}{\partial \mathbf{u}} = \frac{\partial L}{\partial \dot{\mathbf{x}}} \quad (2.4)$$

which identifies the Lagrange multiplier \mathbf{p} as the generalized momentum defined in Lagrange mechanics. Meanwhile, the variational approach derives the governing equations for \mathbf{x} and \mathbf{p} as

$$\dot{\mathbf{x}} = \frac{\partial H}{\partial \mathbf{p}}, \quad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{x}} \quad (2.5)$$

which can be solved to give the optimal trajectory $\mathbf{x}(t)$ and $\mathbf{p}(t)$.

The optimal control $\mathbf{u}(t) = \dot{\mathbf{x}}(t)$ obtained from the variational approach is a function of time, which is valid only for the system starting from a specified initial state $\mathbf{x}(0)$. This type of optimal control is called open-loop optimal control, because for other initial conditions, the optimal control has to be recomputed accordingly. In 1957, Bellman proposed an alternative approach to optimal control, which is valid for all initial states. Bellman wrote the following in his book [13]: “In place of determining the optimal sequence of decisions from the fixed state of the system, we wish to determine the optimal decision to be made at any state of the system. Only if we know the latter, do we understand the intrinsic structure of the solution”. The approach realizing this idea, known as dynamic programming, leads to necessary as well as sufficient conditions for optimality.

Instead of the problem of minimizing $J(t_0, \mathbf{x}_0, \mathbf{u})$ for given t_0 and \mathbf{x}_0 , the basic idea of dynamic programming is to consider a family of minimization problems associated with the cost functional

$$J(t, \mathbf{x}, \mathbf{u}) = \int_t^{t_f} L(\tau, \mathbf{x}(\tau), \mathbf{u}(\tau)) d\tau, \quad (2.6)$$

where t is the current time, which may be any instant between t_0 and t_f , and $\mathbf{x} = \mathbf{x}(t)$ is the current state. The cost function $J(t, \mathbf{x}, \mathbf{u})$ computes the cost accumulated from the current time t to the terminal time t_f and is recognized as the cost-to-go. The dynamic programming approach aims to find the optimal control $\mathbf{u} = \dot{\mathbf{x}}$ to minimize the cost-to-go $J(t, \mathbf{x}, \mathbf{u})$ for arbitrary current time t and current state \mathbf{x} . Under the action of optimal control, the optimal cost-to-go function is defined as

$$V(t, \mathbf{x}) = \min_{\substack{\mathbf{u}(\tau, \mathbf{x}(\tau)) \\ t \leq \tau \leq t_f}} J(t, \mathbf{x}, \mathbf{u}), \quad (2.7)$$

Bellman showed that the optimal momentum \mathbf{p} achieving the minimum cost function can be expressed analytically as

$$\mathbf{p}(t, \mathbf{x}) = -\frac{\partial V(t, \mathbf{x})}{\partial \mathbf{x}}. \quad (2.8)$$

The most remarkable result of dynamic programming approach is to characterize the partial differential equation satisfied by $V(t, \mathbf{x})$,

$$\frac{\partial V(t, \mathbf{x})}{\partial t} = H(t, \mathbf{x}, \mathbf{p})|_{p=-\partial V/\partial \mathbf{x}}. \quad (2.9)$$

When expressed in terms of the action function $S = -V$, Eq. (2.9) becomes the Hamilton–Jacobi equation, which was originally derived in the 1830s as a consequence of canonical transformation. Bellman derived equation (2.9) in 1957 by the concept of dynamic programming instead of canonical

transformation, and Eq. (2.9) is now commonly referred to as the Hamilton–Jacobi–Bellman (HJB) equation.

In other words, Bellman employed the dynamic programming approach to solve the problem of least action, which was solved traditionally by the variational approach. The variational approach is to find the least action applied between two fixed points (t_0, \mathbf{x}_0) and (t_f, \mathbf{x}_f) , while the dynamic programming approach is to find the least action applied between a fixed initial point (t_0, \mathbf{x}_0) and a varying terminal point (t, \mathbf{x}) , i.e.,

$$S(t, \mathbf{x}) = \min_{\substack{\mathbf{u}(\tau, \mathbf{x}(\tau)) \\ t_0 \leq \tau \leq t}} \int_{t_0}^t L(\tau, \mathbf{x}(\tau), \mathbf{u}(\tau)) d\tau. \quad (2.10)$$

The resulting action function $S(t, \mathbf{x})$ can be evaluated at arbitrary t and \mathbf{x} to give the least action from (t_0, \mathbf{x}_0) to (t, \mathbf{x}) . The comparison of the least action function $S(t, \mathbf{x})$ in Eq. (2.10) with the optimal cost function $V(t, \mathbf{x})$ in Eqs. (2.6) and (2.7) reveals that the time t appears as the upper limit of integration in $S(t, \mathbf{x})$ but as the lower limit in $V(t, \mathbf{x})$. The opposite direction of time integration accounts for the fact that the two partial differential equations governing S and V become identical if we set $S = -V$, as shown in Eq. (2.9).

In comparison with the open-loop optimal control expressed by Eq. (2.5), which gives the optimal time trajectories $\mathbf{x}(t)$ and $\mathbf{p}(t)$ emerging from the specific $\mathbf{x}(0)$ and $\mathbf{p}(0)$, the optimal control given by Eq. (2.8) is a closed-loop strategy, which is solely based on the current time t and the current state \mathbf{x} no matter where the current state emerges from.

In the absence of noise, it can be shown that the open-loop optimal control given by the variational approach and the closed-loop optimal control given by the dynamic programming approach are equivalent. However, in the presence of noise, the variational approach is invalid, because it is no longer possible to predict the unique optimal time trajectories $\mathbf{x}(t)$ and $\mathbf{p}(t)$ for a given initial condition. As to the dynamic programming approach, it remains valid under the action of noise, since its strategy is only relevant to current time and current state. It is this feature that allows the dynamic programming approach to be applicable to both deterministic and stochastic systems. In the following, we will show that quantum mechanics can be derived from the optimal control of a stochastic system by using dynamic programming approach.

When an exogenous noise $d\mathbf{w}$ is applied to the deterministic system (2.1), it becomes a stochastic system

$$d\mathbf{x} = f(t, \mathbf{x}, \mathbf{u}) dt + g(\mathbf{x}, \mathbf{u}) d\mathbf{w}, \quad (2.11)$$

where $\mathbf{w} = [w_1 \ w_2 \ \cdots \ w_n]^T$ is the normalized Wiener process satisfying

$$E(dw_j) = 0, \quad j = 1, 2, \dots, n; \quad E(dw_j dw_k) = \delta_{jk} dt, \quad j, k = 1, 2, \dots, n. \quad (2.12)$$

The stochastic optimal control problem is to find the guidance law $\mathbf{u} = \mathbf{u}(t, \mathbf{x})$ to minimize the cost-to-go function (2.6). However, due to the action of noise, the value of the cost-to-go function is random and only its expectation can be minimized,

$$J(t, \mathbf{x}, \mathbf{u}) = E_{t,x} \left\{ \int_t^{t_f} L(\tau, \mathbf{x}(\tau), \mathbf{u}(\tau)) d\tau \right\}. \quad (2.13)$$

The subscript on the expectation value is to remind us that the expectation is over all stochastic trajectories that start from $\mathbf{x}(t) = \mathbf{x}$.

The optimal cost-to-go function $V(t, \mathbf{x})$ is still defined by Eq. (2.7) but with $J(t, \mathbf{x}, \mathbf{u})$ now given by Eq. (2.13). Following the approach of dynamic programming, the main task is to establish the partial differential equation for $V(t, \mathbf{x})$. For this purpose, we partition the integration in Eq. (2.7) into two parts and rewrite $V(t, \mathbf{x})$ as

$$V(t, \mathbf{x}) = \min_{\substack{\mathbf{u}(\tau, \mathbf{x}(\tau)) \\ t \leq \tau \leq t_f}} E_{t,x} \left\{ \int_t^{t+dt} L(\tau, \mathbf{x}(\tau), \mathbf{u}(\tau)) d\tau + \int_{t+dt}^{t_f} L(\tau, \mathbf{x}(\tau), \mathbf{u}(\tau)) d\tau \right\}. \quad (2.14)$$

According to the definition of $V(t, \mathbf{x})$, the second term in the right-hand side is just the cost-to-go starting from $t + dt$, i.e., $V(t + dt, \mathbf{x}(t + dt))$. Therefore, we obtain a differential equation for $V(t, \mathbf{x})$ as

$$V(t, \mathbf{x}) = \min_{\substack{\mathbf{u}(\tau, \mathbf{x}(\tau)) \\ t \leq \tau \leq t+dt}} E_{t,x} \left\{ V(t + dt, \mathbf{x}(t + dt)) + \int_t^{t+dt} L(\tau, \mathbf{x}(\tau), \mathbf{u}(\tau)) d\tau \right\} \quad (2.15)$$

The optimal control $\mathbf{u}(\tau, x(\tau))$ in Eq. (2.14) has to be determined over the interval $t \leq \tau \leq t_f$, while in Eq. (2.15) only the instantaneous value of $\mathbf{u}(\tau, x(\tau))$ at $\tau = t$ is requested to minimize the cost function as $dt \rightarrow 0$. The optimal cost-to-go function $V(t, \mathbf{x})$ now appears on the both sides of Eq. (2.15). In order to solve $V(t, \mathbf{x})$ from Eq. (2.15), we expand $V(t + dt, \mathbf{x}(t + dt))$ with respect to $V(t, \mathbf{x})$ up to the first order of dt ,

$$\begin{aligned} V(t + dt, \mathbf{x}(t + dt)) &= V(t, \mathbf{x}) + \frac{\partial V(t, \mathbf{x})}{\partial t} dt + \frac{\partial V(t, \mathbf{x})}{\partial \mathbf{x}} d\mathbf{x} \\ &\quad + \frac{1}{2} d\mathbf{x}^T \frac{\partial^2 V(t, \mathbf{x})}{\partial \mathbf{x}^2} d\mathbf{x} + O(dt^2) \end{aligned} \quad (2.16)$$

where $\partial^2 V / \partial \mathbf{x}^2$ denotes the Hessian matrix of V with its (j, k) entry given by $\partial^2 V / \partial x_j \partial x_k$. Substituting the above expansion into Eq. (2.15) and evaluating all the expectations at the instant $\tau = t$ and $\mathbf{x}(\tau) = \mathbf{x}$ as $dt \rightarrow 0$, we obtain the following results:

$$(a) E_{t,x} \left(V(t, \mathbf{x}) + \frac{\partial V(t, \mathbf{x})}{\partial t} dt \right) = V(t, \mathbf{x}) + \frac{\partial V(t, \mathbf{x})}{\partial t} dt \quad (2.17)$$

$$\begin{aligned} (b) E_{t,x} \left(\frac{\partial V(t, \mathbf{x})}{\partial \mathbf{x}} d\mathbf{x} \right) &= \frac{\partial V(t, \mathbf{x})}{\partial \mathbf{x}} E_{t,x} (f(t, \mathbf{x}, \mathbf{u}) dt + g(\mathbf{x}, \mathbf{u}) d\mathbf{w}) \\ &= \frac{\partial V(t, \mathbf{x})}{\partial \mathbf{x}} f(t, \mathbf{x}, \mathbf{u}) dt \end{aligned} \quad (2.18)$$

$$\begin{aligned} (c) E_{t,x} \left[d\mathbf{x}^T \frac{\partial^2 V(t, \mathbf{x})}{\partial \mathbf{x}^2} d\mathbf{x} \right] &= E_{t,x} \left[(f(t, \mathbf{x}, \mathbf{u}) dt + g(\mathbf{x}, \mathbf{u}) d\mathbf{w})^T \frac{\partial^2 V(t, \mathbf{x})}{\partial \mathbf{x}^2} (f(t, \mathbf{x}, \mathbf{u}) dt + g(\mathbf{x}, \mathbf{u}) d\mathbf{w}) \right] \\ &= \left(f^T \frac{\partial^2 V}{\partial \mathbf{x}^2} f \right) dt^2 + 2E_{t,x} \left(d\mathbf{w}^T g^T \frac{\partial^2 V}{\partial \mathbf{x}^2} f dt \right) + E_{t,x} \left(d\mathbf{w}^T g^T \frac{\partial^2 V}{\partial \mathbf{x}^2} g d\mathbf{w} \right) \\ &= \text{tr} \left(g^T \frac{\partial^2 V}{\partial \mathbf{x}^2} g \right) dt + \left(f^T \frac{\partial^2 V}{\partial \mathbf{x}^2} f \right) dt^2 \end{aligned} \quad (2.19)$$

$$(d) E_{t,x} \left[\int_t^{t+dt} L(\tau, \mathbf{x}(\tau), \mathbf{u}(\tau)) d\tau \right] = L(t, \mathbf{x}, \mathbf{u}) dt. \quad (2.20)$$

In the derivation of Eq. (2.18) we have used the statistical properties of the Wiener process as stated in Eq. (2.11). Eq. (2.18) shows that a first-order term of dt appears in the second-order expansion of $d\mathbf{x}$, and this fact explains why we retain the second-order term of $d\mathbf{x}$ in the expansion of $V(t + dt, \mathbf{x}(t + dt))$ in Eq. (2.16).

With the expectations computed by Eq. (2.17) to Eq. (2.20), Eq. (2.15) in the limit of $dt \rightarrow 0$ becomes the stochastic Hamilton–Jacobi–Bellman (HJB) equation [15–17]

$$\begin{aligned} - \frac{\partial V(t, \mathbf{x})}{\partial t} &= \min_{\mathbf{u} \in \mathbb{U}} \left\{ L(t, \mathbf{x}, \mathbf{u}) + \frac{\partial V(t, \mathbf{x})}{\partial \mathbf{x}} f(t, \mathbf{x}, \mathbf{u}) \right. \\ &\quad \left. + \frac{1}{2} \text{tr} \left[g^T(\mathbf{x}, \mathbf{u}) \frac{\partial^2 V(t, \mathbf{x})}{\partial \mathbf{x}^2} g(\mathbf{x}, \mathbf{u}) \right] \right\}, \end{aligned} \quad (2.21)$$

whose solution gives the optimal cost-to-go function $V(t, \mathbf{x})$. The minimization in Eq. (2.21) is taken over the set \mathbb{U} , which comprises all the possible instantaneous values of \mathbf{u} at the current time t . Let $\mathbf{u}^* = \mathbf{u}^*(t, \mathbf{x}, V(t, \mathbf{x}))$ be the optimal \mathbf{u} attaining the minimum involved in Eq. (2.21), where the values of $V(t, \mathbf{x})$ and its derivatives are fixed at the current time t and the current state \mathbf{x} . With \mathbf{u} replaced by $\mathbf{u}^*(t, \mathbf{x}, V(t, \mathbf{x}))$, Eq. (2.21) becomes a partial differential equation for $V(t, \mathbf{x})$,

$$-\frac{\partial V(t, \mathbf{x})}{\partial t} = L(t, \mathbf{x}, \mathbf{u}^*) + \frac{\partial V(t, \mathbf{x})}{\partial \mathbf{x}} f(\mathbf{x}, \mathbf{u}^*) + \frac{1}{2} \text{tr} \left[g^T(\mathbf{x}, \mathbf{u}^*) \frac{\partial^2 V(t, \mathbf{x})}{\partial \mathbf{x}^2} g(\mathbf{x}, \mathbf{u}^*) \right]. \quad (2.22)$$

Once a solution $V^*(t, \mathbf{x})$ is solved from Eq. (2.22), the optimal control is eventually determined as $\mathbf{u}^*(t, \mathbf{x}) = \mathbf{u}(t, \mathbf{x}, V^*(t, \mathbf{x}))$, which gives the optimal control strategy at any instant t and any position \mathbf{x} . For a special choice of $f(t, \mathbf{x}, \mathbf{u})$ and $g(\mathbf{x}, \mathbf{u})$, the above process amounts to an optimal stochastic control approach to quantum mechanics and Eq. (2.22) turns out to be the Schrödinger equation.

Before we discuss the specific application to quantum mechanics, we consider a parallel example to familiarize the above process of optimization. A one-dimensional stochastic system is described by

$$dx = (x + u)dt + \sqrt{v}d\xi \quad (2.23)$$

where $d\xi$ is a Wiener process with mean $\langle d\xi \rangle = 0$ and variance $\langle d\xi^2 \rangle = dt$. The control u is to be determined to minimize the quadratic cost function,

$$J(t, x, u) = E_{t,x} \left\{ \frac{1}{2} \int_t^{t_f} (x^2 + u^2) d\tau \right\}. \quad (2.24)$$

With the replacements $f = x + u$, $g = \sqrt{v}$ and $L = (x^2 + u^2)/2$, the HJB equation (2.21) for the present case becomes

$$-\frac{\partial V(t, x)}{\partial t} = \min_{u \in \mathbb{U}} \left\{ (x^2 + u^2)/2 + \frac{\partial V(t, x)}{\partial x} (x + u) + \frac{v}{2} \frac{\partial^2 V(t, x)}{\partial x^2} \right\}. \quad (2.25)$$

The control u minimizing the sum within the brace is found as

$$u^* = -\frac{\partial V(t, x)}{\partial x} \quad (2.26)$$

which in turn is substituted back into Eq. (2.25) to form a partial differential equation for $V(t, x)$,

$$-\frac{\partial V}{\partial t} = \frac{v}{2} \frac{\partial^2 V}{\partial x^2} - \frac{1}{2} \left(\frac{\partial V}{\partial x} \right)^2 + x \frac{\partial V}{\partial x} + \frac{x^2}{2}. \quad (2.27)$$

According to the structure of the above equation, the solution of $V(t, x)$ assumes the following form

$$V(t, x) = \frac{1}{2} p(t)x^2 + \alpha(t)x + \beta(t). \quad (2.28)$$

Substituting this solution into Eq. (2.27) and equating the coefficients of the same powers of x on the both sides, we obtain the governing equations for $p(t)$, $\alpha(t)$ and $\beta(t)$ as

$$\dot{p} = p^2 - 2p - 1, \quad \dot{\alpha} = p\alpha - \alpha, \quad \dot{\beta} = (-vp + \alpha^2)/2. \quad (2.29)$$

The optimal control is synthesized by combining Eqs. (2.26) and (2.28) as

$$u(t, x) = -\frac{\partial V(t, x)}{\partial x} = -p(t)x - \alpha(t) \quad (2.30)$$

where the time functions $p(t)$ and $\alpha(t)$ are solved from Eq. (2.29). The same procedures adopted in this example will be used in the next section to derive quantum mechanics with a different choice for f , g and L .

3. Optimal quantum guidance law

Quantum mechanics is a consequence of the above optimal control design for the stochastic system (2.11) with $f(\mathbf{x}, \mathbf{u}) = \mathbf{u}$ and $g(\mathbf{x}, \mathbf{u}) = \sqrt{\nu}I$, i.e.,

$$d\mathbf{x} = \mathbf{u}dt + \sqrt{\nu}d\mathbf{w}, \quad (3.1)$$

where ν is a diffusion coefficient to be assigned. Taking expectation of both sides of Eq. (3.1) with the property $E(d\mathbf{w}) = 0$, we have $\dot{\mathbf{x}} = \mathbf{u}$. In other words, the guidance command \mathbf{u} determines the mean velocity of the particle so as to minimize the cost function (2.13). With the replacements $f(\mathbf{x}, \mathbf{u}) = \mathbf{u}$ and $g(\mathbf{x}, \mathbf{u}) = \sqrt{\nu}I$, the stochastic HJB equation (2.21) appears as

$$-\frac{\partial V(t, \mathbf{x})}{\partial t} = \min_{\mathbf{u} \in \mathbb{U}} \left\{ L(t, \mathbf{x}, \mathbf{u}) + (\nabla V(t, \mathbf{x}))^T \mathbf{u} + \frac{\nu}{2} \nabla^2 V(t, \mathbf{x}) \right\}. \quad (3.2)$$

The optimal \mathbf{u} achieving the minimum inside the brace for fixed t and \mathbf{x} is determined by the condition

$$\frac{\partial L(t, \mathbf{x}, \mathbf{u})}{\partial \mathbf{u}} = -\nabla V(t, \mathbf{x}). \quad (3.3)$$

We recall that the right-hand-side terms in Eq. (3.2) have been evaluated by taking expectation and the relations $\dot{\mathbf{x}} = \mathbf{u}$ and $L(t, \mathbf{x}, \mathbf{u}) = L(t, \mathbf{x}, \dot{\mathbf{x}})$ have been applied. In the case of quantum mechanics, the instantaneous cost rate $L(t, \mathbf{x}, \dot{\mathbf{x}})$ is chosen as the Lagrangian of the particle. With this particular choice of $L(t, \mathbf{x}, \dot{\mathbf{x}})$, the mean momentum of the particle is given by its definition in Lagrange mechanics

$$\mathbf{p} = \frac{\partial L(t, \mathbf{x}, \dot{\mathbf{x}})}{\partial \dot{\mathbf{x}}}. \quad (3.4)$$

The combination of Eqs. (3.3) and (3.4) yields an expression of \mathbf{p} in terms of the optimal cost-to-go function $V(t, \mathbf{x})$ as

$$\mathbf{p} = \frac{\partial L(t, \mathbf{x}, \dot{\mathbf{x}})}{\partial \dot{\mathbf{x}}} = \frac{\partial L(t, \mathbf{x}, \mathbf{u})}{\partial \mathbf{u}} = -\nabla V(t, \mathbf{x}), \quad (3.5)$$

from which the optimal guidance command \mathbf{u}^* can be determined as a function of t , \mathbf{x} and \mathbf{p} ,

$$\mathbf{u}^* = \mathbf{u}(t, \mathbf{x}, \mathbf{p})|_{p=-\nabla V}. \quad (3.6)$$

Further simplification can be made by introducing the Hamiltonian

$$H(t, \mathbf{x}, \mathbf{p}) = \mathbf{p}^T \dot{\mathbf{x}} - L(t, \mathbf{x}, \dot{\mathbf{x}}) = \mathbf{p}^T \mathbf{u} - L(t, \mathbf{x}, \mathbf{u}). \quad (3.7)$$

With the substitutions of optimal \mathbf{u} from Eq. (3.5) and the Hamiltonian from Eq. (3.7), the Stochastic HJB equation (3.2) turns out to be

$$\frac{\partial S}{\partial t} + H(t, \mathbf{x}, \mathbf{p})|_{p=\nabla S} + \frac{\nu}{2} \nabla^2 S = 0, \quad (3.8)$$

where S is the action function defined as

$$S(t, \mathbf{x}) = -V(t, \mathbf{x}). \quad (3.9)$$

For a particle with mass m moving under the action of a potential $U(t, \mathbf{x})$, the Lagrangian $L(t, \mathbf{x}, \dot{\mathbf{x}})$ has a simple expression:

$$L(t, \mathbf{x}, \dot{\mathbf{x}}) = \frac{m}{2} \dot{\mathbf{x}}^T \dot{\mathbf{x}} - U(t, \mathbf{x}), \quad \mathbf{p} = \frac{\partial L(t, \mathbf{x}, \dot{\mathbf{x}})}{\partial \dot{\mathbf{x}}} = m\dot{\mathbf{x}}. \quad (3.10)$$

The corresponding Hamiltonian $H(t, \mathbf{x}, \mathbf{p})$ defined in Eq. (3.7) reads

$$H(t, \mathbf{x}, \mathbf{p}) = \frac{1}{2m} \mathbf{p}^T \mathbf{p} + U(t, \mathbf{x}). \quad (3.11)$$

According to the value assigned to the constant ν , Eq. (3.8) has three different physical meanings.

(A) $\nu = 0$:

Eq. (3.8) for this case gives the familiar result

$$\frac{\partial S(t, \mathbf{x})}{\partial t} + H(t, \mathbf{x}, \mathbf{p})|_{\mathbf{p}=\nabla S} = \frac{\partial S}{\partial t} + \frac{1}{2m} (\nabla S)^T (\nabla S) + U(t, \mathbf{x}) = 0, \quad (3.12)$$

which is the classical Hamilton–Jacobi (H–J) equation. For this case, the above derivation amounts to the dynamic programming approach to classical mechanics [17].

(B) $\nu \neq 0, \nu \in \mathbf{R}$:

The transformation $S(t, \mathbf{x}) = m\nu \ln \Phi(t, \mathbf{x})$ leads Eq. (3.8) to

$$\frac{\partial \Phi}{\partial t} = \alpha \nabla^2 \Phi - \mu \Phi, \quad (3.13)$$

which is a heat diffusion equation for the temperature difference $\Phi = T - T_s$ with surrounding temperature T_s , thermal diffusivity $\alpha = -\nu/2$ and radiation loss $\mu\Phi = (U/m\nu)\Phi$.

(C) $\nu \neq 0, \nu \in \mathbf{C}$:

This is the case corresponding to quantum motion. The specific value of the complex ν to be considered is

$$\nu = -i\hbar/m, \quad (3.14)$$

where \hbar is Planck constant. The significance of this complex diffusion coefficient, which appeared earlier in the works of Fürth [6] and Comisar [9], lies in its connection between the stochastic HJB equation and Schrödinger equation. Inserting this value of ν into Eq. (3.8), we obtain a quantum version of the classical H–J equation (3.12)

$$\frac{\partial S}{\partial t} + \frac{1}{2m} (\nabla S)^T (\nabla S) + U(t, \mathbf{x}) - \frac{i\hbar}{2m} \nabla^2 S = 0. \quad (3.15)$$

With a further transformation

$$S(t, \mathbf{x}) = -i\hbar \ln \Psi(t, \mathbf{x}), \quad (3.16)$$

we obtain the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + U(t, \mathbf{x})\Psi. \quad (3.17)$$

Up to this stage, we have proved that Schrödinger equation, the kernel equation in quantum mechanics, is just the stochastic HJB equation (2.21) when we solve a stochastic optimal guidance problem described by Eq. (2.11) with $f(\mathbf{x}, \mathbf{u}) = \mathbf{u}$, $g(\mathbf{x}, \mathbf{u}) = \sqrt{-i\hbar/mI}$ and $L = (m/2)\dot{\mathbf{x}}^T \dot{\mathbf{x}} - U(t, \mathbf{x})$. In terms of the Schrödinger's ansatz (3.16), we obtain an interesting link between the optimal cost function $V(t, \mathbf{x})$ and the wavefunction $\Psi(t, \mathbf{x})$:

$$V(t, \mathbf{x}) = i\hbar \ln \Psi(t, \mathbf{x}) \quad (3.18)$$

which symbolizes the proposed interpretation of quantum mechanics as an optimal control problem.

The next issue is to clarify the relation between the optimal guidance law \mathbf{u} and the wavefunction $\Psi(t, \mathbf{x})$ and to confirm the de Broglie–Bohm postulate that $\Psi(t, \mathbf{x})$ is the pilot wave guiding the motion of a quantum particle. The optimal guidance command \mathbf{u} , which determines the mean velocity of the particle, is given by Eqs. (3.5) and (3.10)

$$\mathbf{u} = \dot{\mathbf{x}} = \frac{\mathbf{p}}{m} = -\frac{1}{m} \frac{\partial V(t, \mathbf{x})}{\partial \mathbf{x}} = \frac{1}{m} \frac{\partial S(t, \mathbf{x})}{\partial \mathbf{x}} = -\frac{i\hbar}{m} \frac{1}{\Psi} \frac{\partial \Psi(t, \mathbf{x})}{\partial \mathbf{x}}. \quad (3.19)$$

As expected, the particle's mean velocity is truly guided by the wavefunction $\Psi(t, \mathbf{x})$. The guidance law (3.19) reproduces Bohm's postulate (1.1) from the viewpoint of stochastic optimal guidance law design. However, the two guidance laws given by Eqs. (1.1) and (3.19) are not exactly the same due to their slight difference in the definition of function S . In Eq. (1.1), S_B is a real function determined by the

phase part of $\Psi = R_B(t, \mathbf{x})e^{iS_B(t,\mathbf{x})/\hbar}$, while in Eq. (3.19), S is a complex function related to the complex wavefunction via $\Psi = e^{iS(t,\mathbf{x})/\hbar}$. In the literature, Eq. (3.19) was derived alternatively by quantum Hamilton mechanics [14,18] and was recognized as a complex version of Bohm's proposal [19]. The real-valued quantum trajectory determined by Eq. (1.1) led to a controversy conclusion that a particle is motionless in all its eigenstates. This difficulty could be conquered by the complex quantum trajectory $\mathbf{x}(t)$ solved from Eq. (3.19), which has been recently developed into a potential computational tool to analyze various quantum effects [20,21].

The complex velocity derived in Eq. (3.19) has a close relation to the Brownian motion addressed by Nelson [8], where the current velocity (mean velocity) \mathbf{v}_N and the osmotic velocity \mathbf{u}_N was introduced in terms of the gradients of two functions S_N and R_N as

$$\mathbf{v}_N = \frac{\hbar}{m} \nabla S_N, \quad \mathbf{u}_N = \frac{\hbar}{m} \nabla R_N. \quad (3.20)$$

Nelson showed that the function formed by $\Psi = e^{R_N+iS_N}$ is a solution to the Schrödinger equation. If the Nelson's twin velocities \mathbf{v}_N and \mathbf{u}_N are combined to form a complex velocity,

$$\mathbf{v}_N - i\mathbf{u}_N = \frac{\hbar}{m} \nabla (S_N - iR_N) = -\frac{i\hbar}{m} \nabla \ln \Psi = \dot{\mathbf{x}}, \quad (3.21)$$

we find that the result is just the complex velocity derived in Eq. (3.19). In other words, the real and imaginary parts of the optimal velocity command $\mathbf{u} = \dot{\mathbf{x}}$ are the twin Brownian velocities ($\mathbf{v}_N, -\mathbf{u}_N$) defined in Nelson's work, and are also identical to the two velocity components ($\dot{\mathbf{v}}, -\dot{\xi}(t)$) as defined in Eq. (1.2) by Bohm [5].

4. Quantum Hamilton mechanics

In the last section we have shown that the quantum motion of a particle is guided by its accompanying pilot wave in an optimal manner such that the guided motion minimizes the Lagrangian cost function in the presence of a stochastic Wiener process. The optimal pilot wave is found to be the wavefunction $\Psi(t, \mathbf{x})$ solved from the Schrödinger equation. Instead of using the optimal guidance approach, the same quantum guidance law has been derived by quantum Hamilton mechanics [14]. In this section we will go one step further to show that even quantum Hamilton mechanics itself can be derived from the proposed stochastic optimal control approach, just as classical Hamilton mechanics could be derived from deterministic optimal control approach.

Our aim is to establish the Hamilton equations of motion under the action of the above optimal guidance law and meanwhile to find a quantum version of the classical Hamiltonian (3.11). The first set of Hamilton equations deals with $\dot{\mathbf{x}}$, which has been derived in Eq. (3.19), while the second set deals with $\dot{\mathbf{p}}$, whose components can be expressed as

$$\frac{dp_k}{dt} = \frac{d}{dt} \frac{\partial S(t, \mathbf{x})}{\partial x_k} = \frac{\partial^2 S(t, \mathbf{x})}{\partial t \partial x_k} + \sum_{j=1}^n \frac{\partial^2 S(t, \mathbf{x})}{\partial x_j \partial x_k} \dot{x}_j, \quad (4.1)$$

where \dot{x}_j is given by Eq. (3.19). As to the first term on the right-hand side, we employ the quantum H-J equation (3.15) to give an expression for $\partial S / \partial t$,

$$\begin{aligned} \frac{\partial^2 S(t, \mathbf{x})}{\partial t \partial x_k} &= \frac{\partial}{\partial x_k} \left[-\frac{1}{2m} \sum_{j=1}^n \left(\frac{\partial S}{\partial x_j} \right)^2 - U(t, \mathbf{x}) + \frac{i\hbar}{2m} \sum_{j=1}^n \frac{\partial^2 S}{\partial x_j^2} \right] \\ &= -\frac{1}{m} \sum_{j=1}^n \frac{\partial^2 S}{\partial x_k \partial x_j} \frac{\partial S}{\partial x_j} - \frac{\partial}{\partial x_k} \left[U(t, \mathbf{x}) - \frac{i\hbar}{2m} \sum_{j=1}^n \frac{\partial^2 S}{\partial x_j^2} \right]. \end{aligned} \quad (4.2)$$

The substitution of Eqs. (3.19) and (4.2) into Eq. (4.1) yields the second set of Hamilton equations

$$\frac{dp_k}{dt} = -\frac{\partial}{\partial x_k} \left[U(t, \mathbf{x}) - \frac{i\hbar}{2m} \sum_{j=1}^n \frac{\partial^2 S}{\partial x_j^2} \right]. \quad (4.3)$$

The inspection of the structure in the Hamilton equations (3.19) and (4.3) motivates us to define the quantum Hamiltonian as

$$\begin{aligned} H_\Psi(t, \mathbf{x}, \mathbf{p}) &= \frac{1}{2m} \mathbf{p}^T \mathbf{p} + U(t, \mathbf{x}) - \frac{i\hbar}{2m} \nabla^2 S(t, \mathbf{x}) \\ &= \frac{1}{2m} \mathbf{p}^T \mathbf{p} + U(t, \mathbf{x}) - \frac{\hbar^2}{2m} \nabla^2 \ln \Psi(t, \mathbf{x}). \end{aligned} \quad (4.4)$$

In terms of H_Ψ , Eqs. (3.19) and (4.3) can be incorporated into a standard form of Hamilton equations

$$\frac{d\mathbf{x}}{dt} = \frac{\partial H_\Psi(t, \mathbf{x}, \mathbf{p})}{\partial \mathbf{p}} = \frac{\mathbf{p}}{m}, \quad (4.5a)$$

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial H_\Psi(t, \mathbf{x}, \mathbf{p})}{\partial \mathbf{x}} = -\frac{\partial}{\partial \mathbf{x}} \left[U(t, \mathbf{x}) - \frac{\hbar^2}{2m} \nabla^2 \ln \Psi(t, \mathbf{x}) \right], \quad (4.5b)$$

This is the closed-loop mean dynamics of a quantum particle under the action of the optimal guidance law. The usage of the notation H_Ψ is to emphasize the dependence of the closed-loop dynamics on the optimal cost function $V = i\hbar \ln \Psi$. This property is also called state-dependence in the terminology of quantum mechanics. For a given quantum state described by the wavefunction Ψ , Eq. (4.5) provides the governing equations for a particle moving in the quantum state Ψ . It appears that besides serving as a probability density function, a solution Ψ to the Schrödinger equation also intrinsically determines a set of Hamilton equations (4.5), which forms a complex dynamical representation of the quantum state Ψ . The last term in Eq. (4.4) is known as the complex quantum potential,

$$Q(\Psi(t, \mathbf{x})) = \frac{\hbar}{2mi} \nabla^2 S(t, \mathbf{x}) = -\frac{\hbar^2}{2m} \nabla^2 \ln \Psi(t, \mathbf{x}). \quad (4.6)$$

It can be seen that without the participation of this quantum potential the quantum Hamilton equation (4.5) reduces to the classical Hamilton equations.

One of the merits of quantum Hamilton mechanics consists in the expression of a quantum operator \hat{A} by its complex representation A via the relation

$$A = \frac{1}{\Psi} \hat{A} \Psi. \quad (4.7)$$

In quantum Hamilton mechanics, every physical quantity A can be expressed as a complex function $A(\mathbf{x}, \mathbf{p})$ of the canonical variables \mathbf{x} and \mathbf{p} satisfying the Hamilton equation (4.5), and its operator representation \hat{A} can be identified from Eq. (4.7). Using this relation, we can give a formal proof of the quantization axiom $\mathbf{p} \rightarrow -i\hbar \nabla$ that governs the critical transition from classical systems to quantum-mechanical systems. The canonical momentum \mathbf{p} has been derived by the optimal guidance law (3.19) as

$$\mathbf{p} = \nabla S = -i\hbar \nabla \ln \Psi = \frac{1}{\Psi} (-i\hbar \nabla) \Psi. \quad (4.8)$$

The comparison of the above equation with the definition $\mathbf{p} = (1/\Psi) \hat{\mathbf{p}} \Psi$ gives the canonical momentum operator as

$$\hat{\mathbf{p}} = -i\hbar \nabla. \quad (4.9)$$

We say that the momentum function $\mathbf{p} = \nabla S = -i\hbar \nabla \ln \Psi$ is the complex representation of the momentum operator $\hat{\mathbf{p}}$. Similarly, the Hamiltonian operator \hat{H} can be determined by its complex representation H_Ψ given by Eq. (4.4),

$$H = \frac{1}{2m} (-i\hbar \nabla \ln \Psi)^2 - \frac{\hbar^2}{2m} \nabla^2 \ln \Psi + U = \frac{1}{\Psi} \left(\frac{-\hbar^2}{2m} \nabla^2 + U \right) \Psi. \quad (4.10)$$

The comparison with the definition $H = (1/\Psi)\hat{H}\Psi$ yields the Hamiltonian operator

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V = \frac{1}{2m}\hat{\mathbf{p}}^2 + V. \quad (4.11)$$

For any complex variable A defined in quantum Hamilton mechanics, we can identify its accompanying operator \hat{A} by using Eq. (4.7). As a representative example, we demonstrate how to obtain the angular momentum operator $\hat{\mathbf{L}}$ from its complex realization \mathbf{L} . In quantum Hamilton mechanics, the expression for $\mathbf{L} = \mathbf{x} \times \mathbf{p}$ is the same as that in classical mechanics but with $\mathbf{x} = [x \ y \ z]$ and $\mathbf{p} = [p_x \ p_y \ p_z]$ satisfying the quantum Hamilton equation (4.5), instead of the classical Hamilton equations. Evaluating the x component of \mathbf{L} with \mathbf{p} given by Eq. (4.8), we obtain

$$L_x = yp_z - zp_y = y\left(\frac{\hbar}{i}\frac{\partial \ln \Psi}{\partial z}\right) - z\left(\frac{\hbar}{i}\frac{\partial \ln \Psi}{\partial y}\right) = -\frac{i\hbar}{\Psi}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\Psi. \quad (4.12)$$

Comparing the above equation with the definition $L_x = (1/\Psi)\hat{L}_x\Psi$ gives

$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) = y\hat{p}_z - z\hat{p}_y, \quad (4.13)$$

where we have used the expressions for \hat{p}_y and \hat{p}_z derived in Eq. (4.9). The other two components $\hat{L}_y = z\hat{p}_x - x\hat{p}_z$ and $\hat{L}_z = x\hat{p}_y - y\hat{p}_x$ can be derived similarly.

5. Quantum trajectories under optimal guidance law

Quantum Hamilton mechanics considers only the mean motion of a quantum particle, because the instantaneous random motion has been averaged out during the process of taking expectation in Eq. (2.13). The actual quantum dynamics is described by the stochastic differential equation (3.1) with optimal guidance command \mathbf{u} given by Eq. (3.19) and v given by Eq. (3.14),

$$dx = u(t, x)dt + \sqrt{v}dw = -\frac{i\hbar}{m}\frac{d \ln \Psi(t, x)}{dx}dt + \sqrt{\frac{\hbar}{2m}}(-1 + i)dw, \quad (5.1)$$

where for notational simplicity only one component of the vector \mathbf{x} is displayed above; equations for remaining components can be expressed in a similar way. Eq. (5.1) indicates that a particle's displacement dx comprises the drift displacement $u(t, x)dt$ and the random diffusion displacement $\sqrt{v}dw$.

Eq. (5.1) defines a Langevin equation, where $u(t, x)$ is in general a nonlinear function of x . We can numerically integrate such a nonlinear Langevin equation by using the Euler–Maruyama method [22] with a fixed time step Δt ,

$$x_{j+1} = x_j - \frac{i\hbar}{m}\frac{d \ln \Psi(t_j, x_j)}{dx}\Delta t + \sqrt{\frac{\hbar}{2m}}(-1 + i)\xi\sqrt{\Delta t}, \quad j = 0, 1, \dots, n, \quad (5.2)$$

where $\sqrt{\Delta t}$ stems from the standard deviation of the Wiener process dw and ξ is a real-valued random variable with standard normal distribution $N(0, 1)$, i.e., $E(\xi) = 0$ and $\sigma_\xi = 1$. The partition of Eq. (5.2) into real and imaginary parts yields two coupled difference equations:

$$\text{Re}(x_{j+1}) = \text{Re}(x_j) + \frac{\hbar}{m}\text{Im}\left(\frac{d \ln \Psi(t_j, x_j)}{dx}\right)\Delta t - \sqrt{\frac{\hbar}{2m}}\xi\sqrt{\Delta t}, \quad j = 0, 1, \dots, n, \quad (5.3a)$$

$$\text{Im}(x_{j+1}) = \text{Im}(x_j) - \frac{\hbar}{m}\text{Re}\left(\frac{d \ln \Psi(t_j, x_j)}{dx}\right)\Delta t + \sqrt{\frac{\hbar}{2m}}\xi\sqrt{\Delta t}, \quad j = 0, 1, \dots, n. \quad (5.3b)$$

Given an initial position x_0 , infinitely many quantum trajectories can be generated by Eq. (5.3) due to the randomness imposed by the random variable ξ . Upon solving Eq. (5.3), the real part and the

imaginary part of x are coupled and have to be solved simultaneously. However, only the real part of x is recorded for later use, because in the probability interpretation of quantum mechanics, x is treated as a real-valued variable. Our aim below is to confirm that the statistical distribution of the real part of the quantum trajectories solved from Eq. (5.3) coincides with the probability density function (PDF) $\Psi^*\Psi$, and at the same time to reveal the physical meanings of the imaginary part of x .

Before we compute the quantum trajectory x_j from Eq. (5.3), the optimal cost function $V(t, x) = -S(t, x) = i\hbar \ln \Psi(t, x)$ has to be solved in advance from the quantum H-J equation (3.15) or from the equivalent Schrödinger equation (3.17). Here we will consider a Gaussian wave oscillating in a harmonic potential $U(x) = (k/2)x^2$. The Schrödinger equation with an initial Gaussian packet

$$\Psi(0, x) = \pi^{-1/4} e^{-p_0^2/2} \exp [-(x - ip_0)^2/2], \quad (5.4)$$

can be solved analytically (in dimensionless form) as

$$\Psi(t, x) = \pi^{-1/4} e^{-p_0^2/2} \exp \left[-\frac{1}{2}(x - ip_0 \cos t)^2 + xp_0 \sin t - \frac{it}{2} - \frac{ip_0^2}{4} \sin(2t) \right]. \quad (5.5)$$

This wavefunction represents a coherent state [23] known for the remarkable property that its mean motion behaves exactly as a classical harmonic oscillator. The probability density functions in the coordinate space and momentum space are given, respectively, by

$$\Psi_x^* \Psi_x(t, x) = \frac{1}{\sqrt{\pi}} e^{-(x-p_0 \sin t)^2}, \quad \Psi_p^* \Psi_p(t, p) = \frac{1}{\sqrt{\pi}} e^{-(p-p_0 \cos t)^2}, \quad (5.6)$$

from which the mean values and the standard deviations of x and p are computed as

$$E(x) = p_0 \sin t, \quad \sigma_x = \sqrt{1/2}; \quad E(p) = p_0 \cos t, \quad \sigma_p = \sqrt{1/2}. \quad (5.7)$$

The above wavefunction-based statistics can be reproduced from the mean quantum dynamics obtained by substituting Eq. (5.5) into Eq. (3.19),

$$\dot{x} = e^{-it} p_0 + ix. \quad (5.8)$$

Solving Eq. (5.8) with initial condition $x(0) = 0 + i\delta$, $\delta \in \mathbb{R}$, yields

$$x_\delta(t) = p_0 \sin t - \delta(\sin t - i \cos t), \quad p_\delta(t) = p_0 \cos t - \delta(\cos t - i \sin t). \quad (5.9)$$

If we let $\delta = 0$ in Eq. (5.9), then the mean quantum dynamics recovers the mean values listed in Eq. (5.7), i.e., $x_0(t) = E(x) = p_0 \sin t$ and $p_0(t) = E(p) = p_0 \cos t$. Subtracting Eq. (5.9) from their mean values, we get the position and momentum uncertainties as

$$\Delta x = |x_\delta(t) - p_0 \sin t| = |\delta|, \quad \Delta p = |p_\delta(t) - p_0 \cos t| = |\delta|. \quad (5.10)$$

The above relation characterizes the physical meanings of the imaginary part $\delta = \text{Im}(x(0))$ as the quantum uncertainty Δx and Δp . The comparison between Eqs. (5.7) and (5.10) indicates that with $\delta = \text{Im}(x(0)) = \sqrt{1/2}$ the probability-based uncertainties σ_x and σ_p , and the trajectory-based uncertainty Δx and Δp become identical. The product of the quantum certainties Δx and Δp yields

$$\Delta x \Delta p = |x_\delta(t) - p_0 \sin t| \cdot |p_\delta(t) - p_0 \cos t| = 1/2, \quad (5.11)$$

which shows that the coherent state achieves the lower bound of the uncertainty principle (in dimensionless form). This is a well-known result proved before by using the PDFs $\Psi_x^* \Psi_x$ and $\Psi_p^* \Psi_p$, but here we obtain the same result by the complex dynamic model for $x(t)$ and $p(t)$.

We have seen that the mean quantum trajectory $x_0(t)$ and the boundary trajectory $x_\delta(t)$ can be solved from the mean quantum dynamics (3.19). On the other hand, actual quantum trajectories are found by solving Eq. (5.3) with wavefunction $\Psi(t, x)$ given by Eq. (5.5). A total of 160,000 random trajectories all starting from $x_0 = 0 + 0i$ are recorded and plotted as the red curves in Fig. 1(a) and (c) for the real part and imaginary part, respectively. The numerical averages of these random trajectories are shown in Fig. 1(b) and (d). For the purpose of comparison, the mean trajectory x_0 determined from Eq. (5.9) is also shown in Fig. 1(a) and (c) as the blue curves. The complete coincidence of the mean

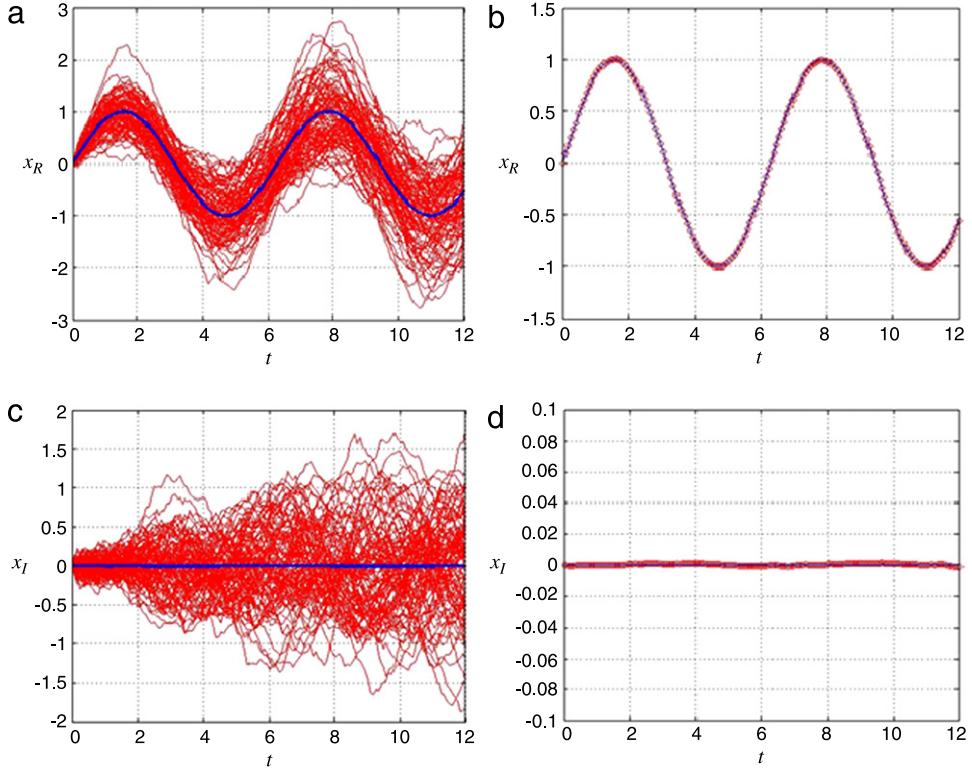


Fig. 1. The real parts (a) and the imaginary parts (c) of 160,000 random trajectories (red curves) solved from Eq. (5.3) for the coherent state. The blue line is the mean trajectory $x_0(t)$ solved from Eq. (5.8) with $x_0 = 0.0 + 0.0i$. The average trajectory obtained by averaging the 160,000 random trajectories coincides with $x_0(t)$ as shown in (b) for the real part and (d) for the imaginary part. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

trajectory x_0 with the numerical average of the random trajectories confirms the fact that the Hamilton equation (4.5) represents the mean dynamics of the random quantum motion described by Eq. (5.1).

Apart from providing a mean trajectory for random quantum motion, a complex trajectory solved from Eq. (5.8) with initial position $x_\delta(0) = 0 + 8i$ can serve as a lower or upper bound for random quantum trajectories. The complex trajectory $x_\delta(t)$ with $\delta = \pm\sigma_x$ satisfying

$$|x_{\pm\sigma}(t) - x_0(t)| = |x_{\pm\sigma}(t) - p_0 \sin t| = \sigma_x = \sqrt{1/2}, \quad (5.12)$$

forms a 1σ -deviation boundary that encompasses 68.26% random trajectories in the coherent state Ψ , as shown in Fig. 2. One hundred and five hundred random paths are generated, respectively, by Eq. (5.3) with $p_0 = 1$. It can be seen that for both cases almost all of the random paths are enveloped by the 3σ boundary curve $x_{\pm 3\sigma}(t)$, which, as expected, is able to cover 99.73% random trajectories. The chromatic level indicates the magnitude of the PDF $\Psi^*\Psi$ whose distribution is consistent with the concentration and dispersion of the random quantum trajectories.

6. Reconstructing PDF by optimal quantum trajectories

We have seen above that a single complex trajectory $x_\delta(t)$ solved from the mean quantum dynamics (3.19) forms a boundary for the quantum uncertainty in Ψ . In this section, we proceed to show that the superposition of an ensemble of complex random trajectories emerging from the same initial position can reproduce the statistical distribution prescribed by $\Psi^*\Psi$. To verify the latter

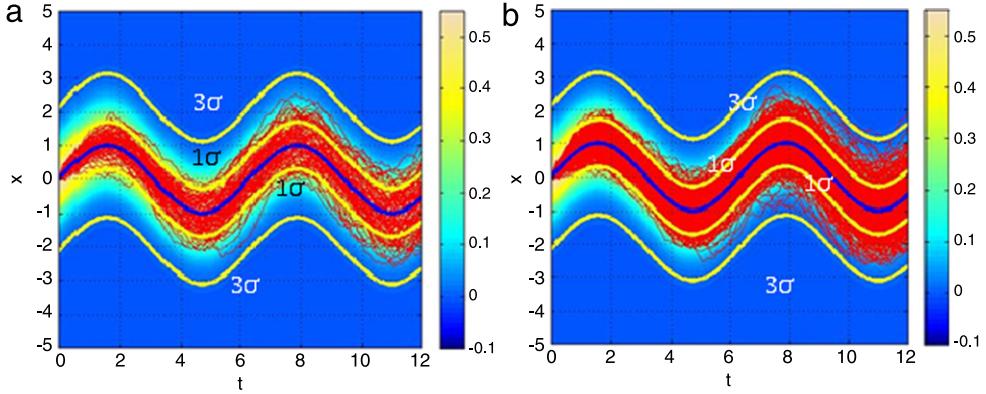


Fig. 2. The boundary of quantum uncertainty for a coherent state with $p_0 = 1$. One hundred (part a) and five hundred (part b) random paths are generated, respectively, by Eq. (5.3) with Ψ given by Eq. (5.5). The 1σ and 3σ deviation boundaries (yellow lines) computed from Eq. (5.9) cover, respectively, 68.26% and 99.73% random quantum paths (red lines). The chromatic level illustrates the magnitude of the PDF $\Psi^*\Psi$ whose value is consistent with the concentration and dispersion of the computed random quantum trajectories. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

meaning of $x(t)$ via the example of the coherent state, we construct the point set $\{\text{Re}(x_j)\}$, which contains N complex trajectories x_j solved from Eq. (5.3), and then compare the statistical distribution of this point set with the distribution of $\Psi^*(t, x)\Psi(t, x)$ given by Eq. (5.6). Different sizes of ensemble of the trajectories with $N = 100, 1000, 10,000$ and $100,000$ are used to construct the point set $\{\text{Re}(x_j)\}$, whose spatial distributions at the instant $t = 10.8$ are shown in Fig. 3. It can be seen that as the size of the ensemble increases, the spatial distribution of the point set $\{\text{Re}(x_j)\}_{t=10.8}$ converges gradually to the distribution of the PDF $\Psi^*(t, x)\Psi(t, x)$ evaluated at $t = 10.8$.

It is noted that all the random trajectories here emerge from the same initial position $x(0) = 0 + 0i$. By contrast, the quantum trajectories considered in the existing literature start from different initial positions whose distribution is deliberately selected in order to generate an ensemble of trajectory compatible with $\Psi^*(t, x)\Psi(t, x)$. The stochastic differential equation (5.1) derived from the optimal guidance approach automatically generates compatible trajectories no matter how the initial positions of the trajectories are prepared.

To quantify the matching error between the position distributions of $\{\text{Re}(x_j)\}$ and the PDF $\Psi_x^*(t, x)\Psi_x(t, x)$, $x \in \mathbf{R}$, the correlation coefficient Γ between them is calculated,

$$\Gamma = \frac{S_{AB}}{\sqrt{S_{AA}S_{BB}}}, \quad -1 \leq \Gamma \leq 1, \quad (6.1)$$

where

$$S_{AA} = \sum_{j=1}^n (A_j - \bar{A})^2, \quad S_{BB} = \sum_{j=1}^n (B_j - \bar{B})^2, \quad S_{AB} = \sum_{j=1}^n (A_j - \bar{A})(B_j - \bar{B}), \quad (6.2)$$

with data A_j obtained from the point set $\{\text{Re}(x_j)\}$ and B_j from the PDF $\Psi_x^*\Psi_x$. We can see from Fig. 3 that the correlation coefficient approaches to 1 as the size of the trajectory ensemble increases.

The spatial distributions of $\{\text{Re}(x_j)\}$ observed at six instants $t = 2, 4, 6, 8, 10$ and 12 with a fixed size of ensemble $N = 100,000$ are shown in Fig. 4. Because all the trajectories start from the same initial point $x_0 = 0 + 0i$, in the beginning the trajectories do not fully disperse over the real axis and the initial distribution of $\{\text{Re}(x_j)\}$ is very different from the distribution of $\Psi_x^*\Psi_x$ (green line in Fig. 4). As time proceeds, enough spatial points are reached by the trajectories so that the distribution of $\{\text{Re}(x_j)\}$ gradually evolves into a fixed pattern identical to $\Psi_x^*\Psi_x$.

The Wiener process w in the stochastic differential equation (5.1) is critical to the guidance interpretation of quantum mechanics. It tells us how to generate the noise such that the resulting random

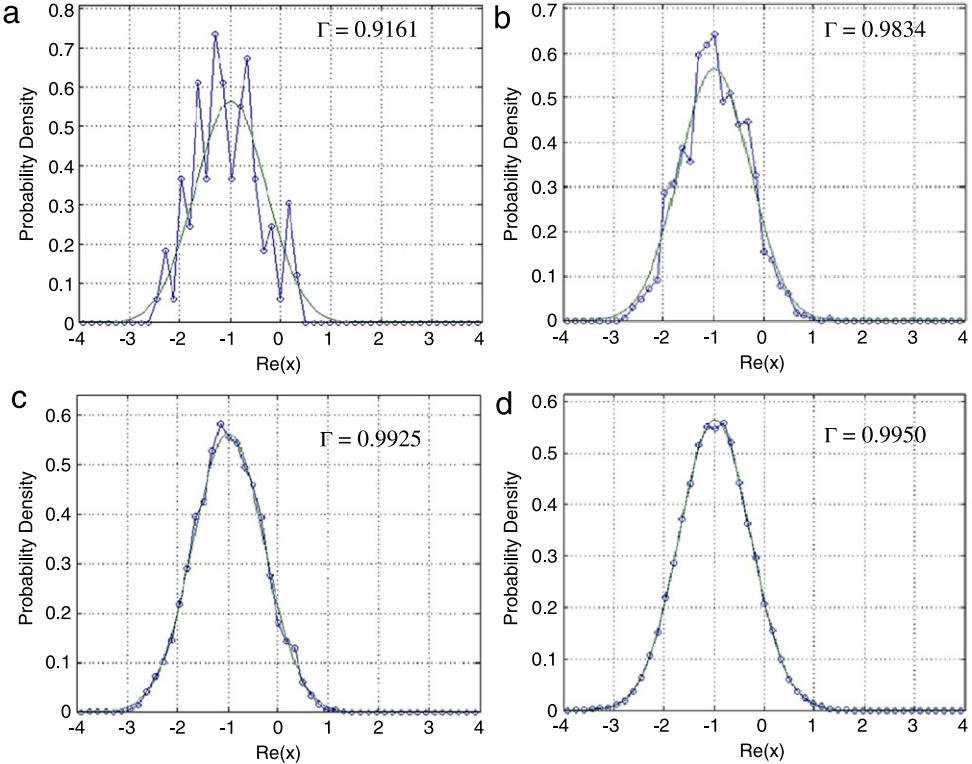


Fig. 3. The reproduction of $\Psi^* \Psi$ (green line) for a Gaussian wave packet with harmonic oscillation at the instant $t = 10.8$ by different numbers of trajectories (blue lines): (a) 100, (b) 1000, (c) 10,000, and (d) 100,000. All the random trajectories emerge from the same initial position $x(0) = 0 + 0i$. The computed correlation coefficient Γ shows that a large enough ensemble of trajectories is required to reproduce the statistical property of $\Psi^* \Psi$ correctly. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

trajectories can reproduce the statistical property of Ψ . In Eq. (5.2), the random variable ξ is added to the iteration at every time step Δt . As $\Delta t \rightarrow 0$, the trajectory becomes fractal and non-differentiable everywhere. For the purpose of comparison, we remove the Wiener process from Eq. (5.1) to see whether the remaining deterministic differential equation, i.e., Eq. (3.19), can produce quantum motion consistent with the description of the wavefunction Ψ . A straightforward discretization of Eq. (3.19) yields

$$x_{j+1} = x_j - \frac{i\hbar}{m} \frac{d \ln \Psi(t_j, x_j)}{dx} \Delta t, \quad j = 0, 1, \dots, n. \quad (6.3)$$

For a given initial position x_0 , only one trajectory can be generated from Eq. (6.3). Uncertainty has to be imposed on x_0 in order to yield an ensemble of deterministic trajectories. The distribution of initial positions is suggested as

$$x_0 = 0 + i\xi \sqrt{\frac{\hbar \Delta t}{2m}}, \quad \xi \approx N(0, 1). \quad (6.4)$$

The real part of x_0 is still fixed at zero, but its imaginary part is now generated by the random variable ξ as suggested by Eq. (5.3b). This arrangement of the initial condition is to reflect the situation, taking place in the quantum world, that even though we have precise information about the initial position $\text{Re}(x_0)$ and the governing equation (6.3), the resulting trajectory is still uncertain due to the influence of the unobservable part $\text{Im}(x_0)$.

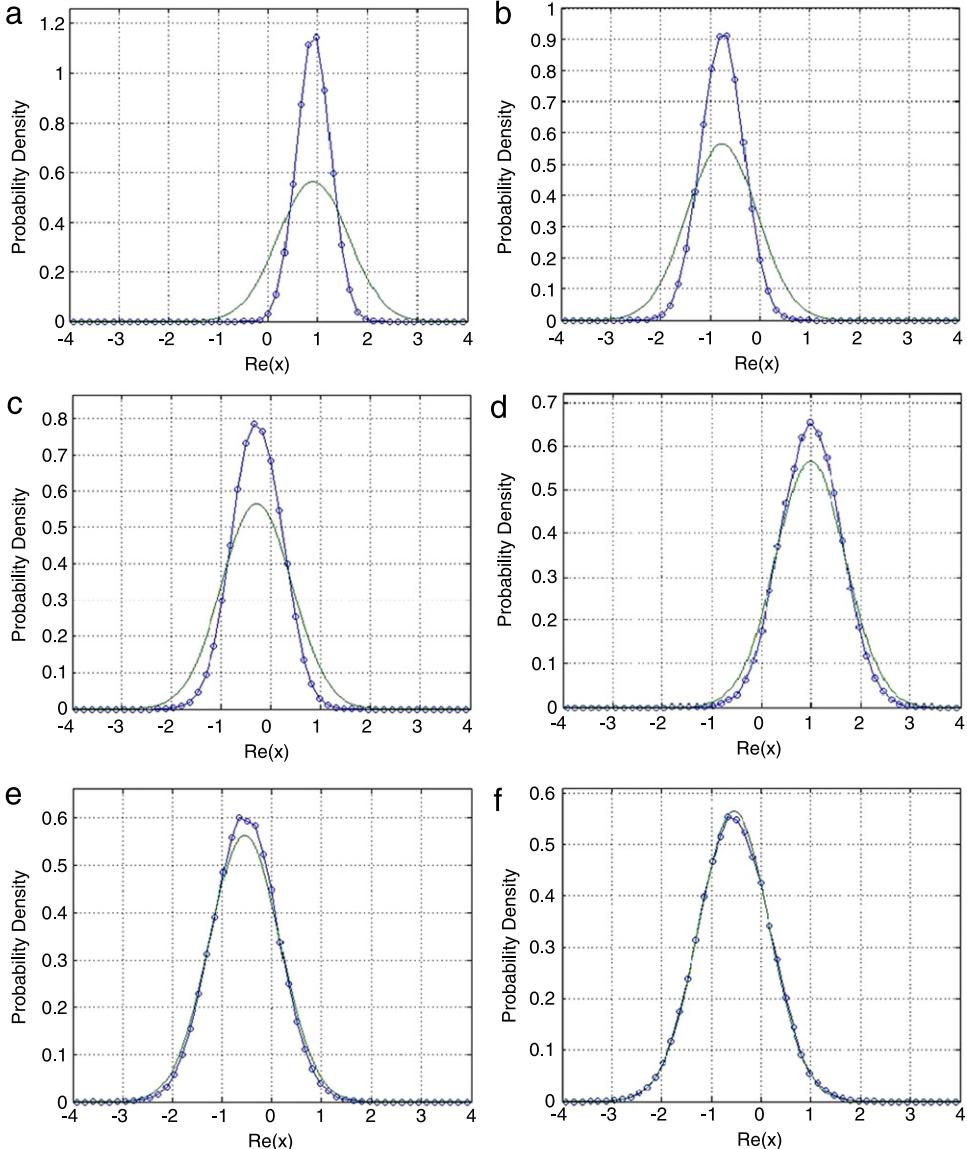


Fig. 4. The reproduction of $\Psi^*\Psi$ for a Gaussian wave packet with harmonic oscillation by 100,000 random trajectories at six time instants (a) $t = 2$, (b) $t = 4$, (c) $t = 6$, (d) $t = 8$, (e) $t = 10$, and (f) $t = 12$. As time evolves, the statistical distribution of the 100,000 trajectories converges to the prediction of $\Psi^*\Psi$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

A total of 100,000 values of $\text{Im}(x_0)$ are selected according to the distribution of ξ and 100,000 deterministic complex trajectories are computed from Eq. (6.3). The point set $\{\text{Re}(x_j)\}$ of the resulting 100,000 trajectories is created and its correlation coefficient $\Gamma_D(t)$ with respect to the PDF $\Psi^*\Psi$ is computed as a function of time as shown in Fig. 5. Also shown in Fig. 5 is the correlation coefficient $\Gamma_R(t)$ based on 100,000 random complex trajectories computed from Eq. (5.3). Although all the random trajectories start from the same position $\text{Re}(x_0) = \text{Im}(x_0) = 0$, the addition of the random variable ξ at every time step diversifies the trajectories quickly so as to develop a statistical pattern

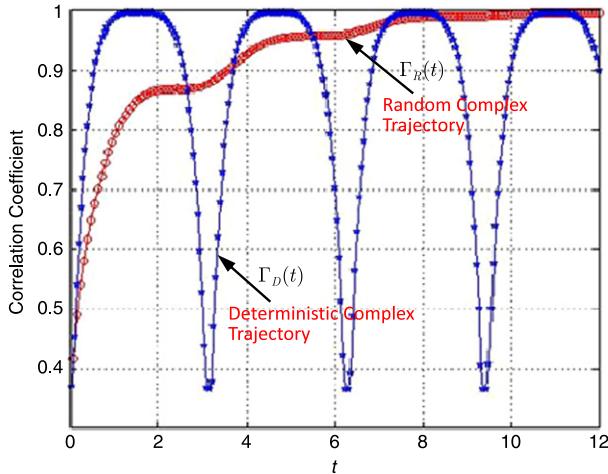


Fig. 5. Time response of two correlation coefficients for a coherent state. The blue line is the correlation coefficient $\Gamma_D(t)$ between the deterministic complex trajectories solved from Eq. (6.3) and the PDF $\Psi^*\Psi$, while the red line is the correlation coefficient $\Gamma_R(t)$ between the random complex trajectories solved from Eq. (5.3) and the PDF $\Psi^*\Psi$. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

approaching to $\Psi^*\Psi$, as is reflected in Fig. 5, where $\Gamma_R(t)$ increases monotonically to 1 as time proceeds. Indeed, the choice of $\text{Re}(x_0)$ is arbitrary; random trajectories solved from Eq. (5.3) are allowed to start with different initial positions without changing the property of convergence $\Gamma_R(t) \rightarrow 1$, as $t \rightarrow \infty$. Especially, if $\text{Re}(x_0)$ is chosen randomly according to the distribution of the initial PDF $\Psi^*\Psi(0, x)$, then we will have a perfect reconstruction of $\Psi^*\Psi(t, x)$ by the point set $\{\text{Re}(x_j)\}$ at any instant, i.e., $\Gamma_R(t) = 1, \forall t \geq 0$.

On the other hand, the correlation coefficient $\Gamma_D(t)$ constructed from the deterministic model has a periodic oscillation as shown in Fig. 5, being unable to reach a steady value at 1. The periodic nature of $\Gamma_D(t)$ originates from the deterministic equation (6.3), whose solutions lose diversity in the beginning and in the end of each period of motion, where all the trajectories start from or converge to the same point $\text{Re}(x_0) = 0$. In summary, the deterministic dynamics given by Eq. (3.19) or Eq. (6.3) is helpful to determine mean quantum motion and to estimate the boundary of quantum uncertainty. As long as the actual quantum trajectory is concerned, the Wiener process dw has to be superposed on the deterministic dynamics to form the stochastic differential equation (5.1), whose solutions automatically manifest the statistic behavior prescribed by the PDF $\Psi^*\Psi$, no matter what the initial positions are. The stochastic differential equation (5.1), which is derived in this paper by the approach of stochastic optimal guidance design, serves as a complex representation of the quantum state Ψ , which reveals the internal mechanism underlying the externally observed PDF $\Psi^*\Psi$.

7. Conclusions

In this paper, de Broglie's pilot wave idea is proved and realized by stochastic optimal guidance design for an equivalent guidance problem within which a quantum particle is regarded as the flight vehicle to be guided and its accompanying pilot wave is the guidance law to be designed so as to guide the particle to a random target driven by a stochastic Wiener process, while minimizing the Lagrangian cost function. Several significant findings have been revealed by this innovative interpretation of quantum mechanics.

1. The Schrödinger equation is just the stochastic Hamilton–Jacobi–Bellman (HJB) equation arising from solving the proposed optimal control problem by a dynamic programming approach, and the optimal guidance law (the pilot wave) is synthesized by the wavefunction $\Psi(t, x)$, a solution to the Schrödinger equation.

2. The quantum noise is engaged to the guidance system via a complex gain $\sqrt{-i\hbar/m}$ so that the closed-loop quantum guidance system can be represented by a complex state-space model from which quantum operators emerge automatically.
3. A quantum displacement contains two components. The deterministic component is called drift displacement which is driven by the optimal guidance command. The random component is called diffusion displacement which is driven by a Wiener process. The former characterizes the mean and variance of quantum trajectories, while the latter contributes randomness and fractal to quantum trajectories.
4. The optimal guidance approach to quantum mechanics yields a stochastic differential equation, from which quantum trajectories can be solved and visualized with any given resolution. The statistical distribution of the resulting quantum trajectories is shown to consist with the prediction of the probability density function $\Psi^*\Psi$. In other words, the random trajectories solved from Eq. (5.1) actually give an explicit characterization of the quantum paths proposed by Feynman in his path integral approach to quantum mechanics.

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